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Imperfect 2D phosphorus, yet an almost perfect semiconductor EVGENI PENEV, YUANYUE LIU[1], FANGBO XU, ZIANG ZHANG, BORIS YAKOBSON, Rice Univ — The deep gap states created by defects in semiconductors typically deteriorate the performance of (opto)electronic devices. This has limited the applications of two-dimensional (2D) metal dichalcogenides (MX_2) and underscored the need for a new 2D semiconductor without defect-induced deep gap states. The talk will discuss why a 2D mono-elemental semiconductor can be a promising candidate. This is exemplified by a first-principles study of 2D phosphorus ("phosphorene") [1], a recently fabricated high-mobility semiconductor. Most of the defects, including intrinsic point defects and grain boundaries, are electronically inactive, thanks to the homoelemental bonding, which is not preferred in heteroelemental system such as MX_2. Unlike MX_2, where the edges create deep gap states and cannot be eliminated by passivation, the edge states of 2D P can be removed from the band gap by hydrogen termination. It is further found that both the type and the concentration of charge carriers in 2D P can be tuned by doping with foreign atoms. The work sheds light on the role of defects on the electronic structure of low-dimensional materials in general.

[1] Y. Liu, F. Xu, Z. Zhang, E. S. Penev, and B. I. Yakobson, Nano Lett. (2014), DOI: 10

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